

Scaling of cluster fluctuations in two-dimensional $q = 5$ and 7 state Potts models[†]

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Abstract

The scaling behavior of fluctuations in cluster size is studied in $q = 5$ and 7 state Potts models. This quantity exhibits scaling behavior on small lattices where the scaling of local operators like energy fluctuations and Binder cumulant can not be expected.

Keywords: First-order phase transition, Potts model, finite size scaling, Monte Carlo simulation

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Rigorous theory of finite size scaling, for first-order phase transitions, put forward by Borg et. al. [1, 2] gave explicit form for the size dependence of various operators. According to this theory, for periodic boundary conditions, the operators such as specific heat and Binder cumulant at the transition temperature can be represented by a polynomial in $1/L^d$ where L is the linear lattice size and d is the dimension. If the lattice sizes are much larger than the correlation length, the contribution of the higher order terms are negligible [3]. The difficulty arises when the correlation length is of the order of the lattice size or larger. In this case, higher order corrections are necessary and deciding the order of the transition becomes difficult. Even when the large lattices are used, higher order terms may create difficulties during the fitting process to the simulation data. Such difficulties may be reduced by choosing the operators for which the correction terms play less important role. A good example for such an operator is the average energy measured at the infinite lattice transition point. This quantity has exponentially small correction term which enables one to determine the infinite lattice critical point with great accuracy [2, 3, 4].

In an earlier work [6, 7] on the two-dimensional Potts model, it is observed that compared to the local operators such as energy and order parameter, cluster related (global) operators are more sensitive to the changes in the system going through a phase transition. Particularly, the average cluster size distribution may give better indication on the order of the phase transition at smaller sizes than that for the en-

ergy distribution. The most trustworthy method to test this observation is studying the finite size scaling behavior of the cluster related operators. In this work, the finite size behavior of the cluster size fluctuations in q -state Potts model under the light of the finite size scaling theory, developed for first-order phase transitions in the past decade [1,2,7,8] will be examined.

The two-dimensional q -state Potts model is known to undergo a first-order phase transition for $q > 4$ [8]. While the correlation length at this transition, ξ , is about 10 lattice sites for $q = 10$, ξ approaches infinity in the limit as $q \rightarrow 4$, [9]. Even though the $q = 7$ Potts model exhibits strong first-order behavior, correlation length is of the order of 50 lattice sites. $q = 5$ state model has a weak first-order transition with a correlation length about few thousand in lattice units. In various studies on finite size scaling behavior of the q -state Potts model, it has been shown that $q \geq 10$ state Potts model enters into asymptotic regime for the lattice sizes $L > 40$ [4, 5, 12] (for a review see [3]). This makes the observation of scaling difficult for $q < 10$ in simulation studies by using computationally feasible lattice sizes [4, 13, 14] where higher order corrections become important. However these studies are based on the finite size scaling behavior of the local operators such as the energy cumulants. The aim in this work is to observe the characteristic behaviours in the system by studying global operators such as fluctuations in cluster size which may yield information on the scaling form of the operators and hence on the order of the transition.

The Hamiltonian of the Potts model [15, 16] is given by

$$-\beta\mathcal{H} = K \sum_{\langle i,j \rangle} \delta_{\sigma_i, \sigma_j}. \quad (1)$$

Here $K = J/kT$; where k and T are the Boltzmann constant and the temperature respectively, and J is the magnetic interaction between spins σ_i and σ_j , which can take values $1, 2, \dots, q$ for the q -state Potts model. One of the basic operators, the average cluster size can be defined as

$$ACS = \frac{1}{N_C} \langle \sum_{i=1}^{N_C} C_i \rangle \quad (2)$$

where C_i is the number of spins in the i^{th} cluster divided by the total number of spins. Similar to the energy cumulants, the fluctuations in this quantity at the transition temperature take a polynomial form [1]

$$(\langle C^2 \rangle - \langle C \rangle^2)_{max} = A_0 + A_1/L^d + A_2/L^{2d} + \dots \quad (3)$$

where d is the space dimension.

In the simulation of 7-state Potts model the measurements are done on twelve lattices in the range $12 \leq L \leq 64$. Since the calculated correlation length ξ of this model is about 50 lattice sites [9], this set of lattices are considered to be an indicative set for both very small lattice measurements and for the lattices of the order of the correlation length. Measurements are done around the transition temperature and

at each temperature 5×10^5 iterations are performed following the thermalization runs of 5×10^4 to 10^5 iterations. For $q = 5$ state Potts model, the measurements are done on lattice $32 \leq L \leq 128$. On the largest three lattices 10^6 iterations were performed in order to obtain the same statistical errors. For all simulation works, cluster update algorithm [10, 11] is employed.

The first indication towards the realization of our expectations of the scaling behavior of cluster related operators can be seen in Fig. 1 where cluster size fluctuation (FCS) data for $q = 7$ model is displayed. Using only the lattices with $48 \leq L$, the cluster size fluctuations (FCS) data exhibit *data collapsing* which is a manifestation of scaling. Furthermore, as one can see from Fig. 1, the data obtained on lattices $28 \leq L \leq 48$, deviate very little around the data collapse curve which means a possible correction term in scaling form has very little effect. This is an indication that the asymptotic regime is reached for these lattices. Such a data collapse for $L \leq 64$ is impossible to observe for the energy fluctuations, as it has been studied extensively in literature [4]. This observation is also supported by the fits done to the maxima of the cluster fluctuation data $(FCS)_{max}$. This quantity is expected to be independent of size in the scaling region for a strong first-order phase transition. In Fig. 2, the $(FCS)_{max}$ values are plotted against $1/L^d$. The $(FCS)_{max}$ of the largest three lattices ($L=48, 56$ and 64), in most conservative view, are size independent. Increasing the number of data points by considering the next two lattices

gives the same constant within errors and improves the quality of the fit. The fit can be repeated by including smaller size lattices ($L \leq 40$) in which case the first correction term in Eq. (3) must be included (FORM1 = $A_0 + A_1/L^d$). When all the lattice sizes are included, the results are $A_0 = 0.0843 \pm 0.0003$ and $A_1 = 0.630 \pm 0.064$ with $\chi^2 = 0.43$. The third term in Eq. (3) seems to have no effect on the first two coefficients and the large error on the coefficient A_2 indicates that this term has no room for this set of data.

In the case of 5-state Potts model, since the correlation length is of the order of few thousands of spins, observing asymptotic behavior by using lattices of size in the range of $L = 32$ to 128 sites can not be expected. Nevertheless, if one can see the expected finite size behavior with the correction terms, this can be indicative of the order of the transition. Fig. 3 shows $(FCS)_{max}$ versus $1/L^d$ for $q = 5$ Potts model. A linear fit in $1/L^d$ (FORM1) to the largest four lattices ($64 \leq L$) gives $A_0 = 0.0429 \pm 0.0007$ and $A_1 = 48.1 \pm 5.7$ with $\chi^2 = 0.16$. For a fit to the smaller lattices, A_2/L^{2d} term becomes necessary (FORM2 = $A_0 + A_1/L^d + A_2/L^{2d}$). This form fits to the lattices between size 128 down to 56. In this procedure A_0 and A_1 remains unchanged within the error bars. In order to include smaller lattices another form (FORM3 = $A_0 + A_1/L^d + A_2 \exp(-A_3 L)$) has also been tested for all size lattices. This form fits to all of the lattices (Fig.3.) while leaving the first coefficient (A_0) unchanged.

Recently there has been a new publication in support of the idea that the global operators carry more information than the local operators [17]. The finite size scaling algorithm based on bulk and surface renormalization of de Oliveira [18] is tested on q -state Potts models in dimensions $d = 2$ and 3 . The operators chosen are very sensitive to the order of the transition. They have calculated the magnetic critical index and obtained with good accuracy the first-order value for even weak first-order transitions such as for the $d = 2$, $q = 5$ Potts model. This is in support of our expectations.

In conclusion, the cluster size fluctuations data for 7-state Potts model on rather moderate size lattices fits to the expected behavior of the first-order phase transitions with scaling exponent being the space dimension. Measurements on lattices as small as $L = 28$ indicate that a very small correction is needed for scaling of the cluster fluctuation peaks. Furthermore, as it is expected from the large correlation length, the $q = 5$ case can not show such good scaling behavior, but nevertheless the expected form for first-order phase transition can be observed with very stable fits to the data. In the case of energy fluctuations, the data collapse, even for the $q=7$ state Potts model case, is seen to be impossible and the lattices considered failed to give even stable fits. In this respect it can be emphasized that the choice of the operators is extremely important, especially in the case of weak first-order phase

transitions. The results are in favor of previous observations that the operators which possess global information on the system can better exhibit the character of the phase transition.

References

- [1] C. Borgs and R. Kotecky, J. Stat. Phys. 61 (1990) 79.
- [2] C. Borgs, R. Kotecky and S. Miracle-Sole, J. Stat. Phys. 62 (1991) 529.
- [3] A. Billoire, Nucl. Phys. (Proc. Suppl.) B42 (1995) 21.
- [4] A. Billoire, R. Lacaze and A. Morel, Nucl. Phys. B370 (1992) 773.
- [5] A. Billoire, Int. J. of Mod. Phys. C3 (1992) 913.
- [6] M. Aydın, Y. Gündüç and T. Çelik, Physica A230 (1996) 651.
- [7] Y. Gündüç, T. Çelik and M. Aydın, Physica A, in press.
- [8] R. J. Baxter, J. Phys. C6 (1973) L445.
- [9] E. Buffenoir and S. Wallon, J. Phys. A26 (1993) 3045.
- [10] R. H. Swendsen and J. S. Wang, Phys. Rev. Lett. 58 (1987) 86.
- [11] U. Wolff, Phys. Rev. Lett. 62 (1989) 361.

- [12] J. Lee and J. M. Kosterlitz, Phys. Rev. B43 (1991) 3265.
- [13] J. Janke, B. Berg and M. Katoot, Nucl. Phys. B382 (1992) 649.
- [14] K. Rummukainen, Nucl. Phys. B390 (1993) 621.
- [15] R. B. Potts, Proc. Camb. Phil. Soc. 48 (1952) 106.
- [16] F. Y. Wu, Rev. Mod. Phys. 54 (1982) 235.
- [17] P.M.C. de Oliveria, S.M. Moss de Oliveria, C.E. Cordeiro and D. Stauffer, J. Stat. Phys. 80 (1995) 1433.
- [18] P.M.C. de Oliveira , Europhys. Lett. 20 (1992) 621.

Figure captions

Figure 1. FCS data versus $(K - K_c) \times L^d$ for $q = 7$ Potts model.

Figure 2. $(FCS)_{max}$ plotted as a function of $\frac{1}{L^d}$ for $q = 7$ Potts model. The lattice sizes are $12 \leq L \leq 64$.

Figure 3. $(FCS)_{max}$ plotted as a function of $\frac{1}{L^d}$ for $q = 5$ Potts model. The lattice sizes are $32 \leq L \leq 128$.

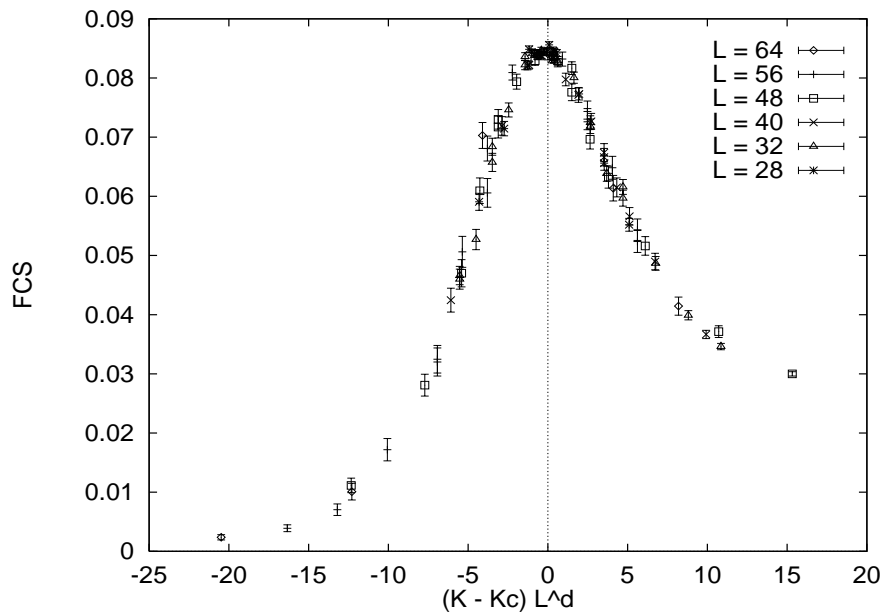


Figure 1:

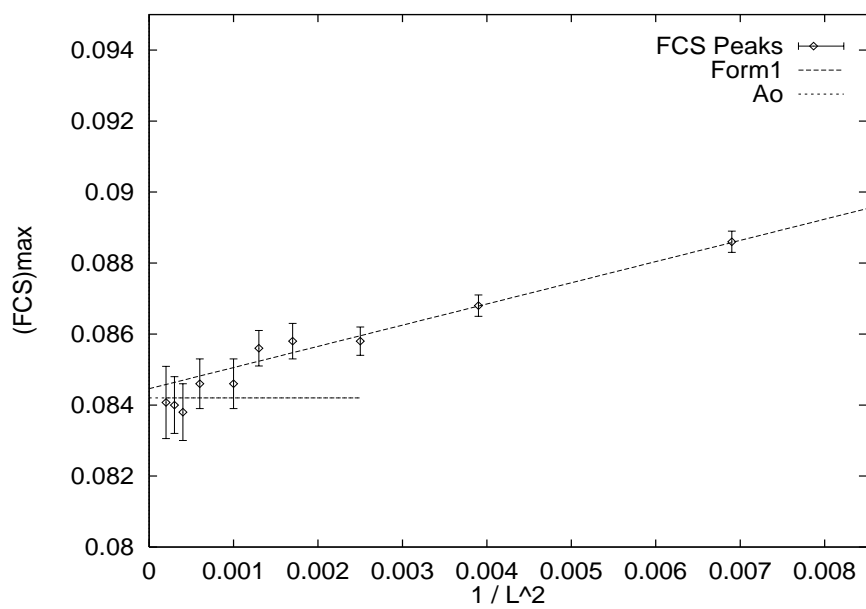


Figure 2:

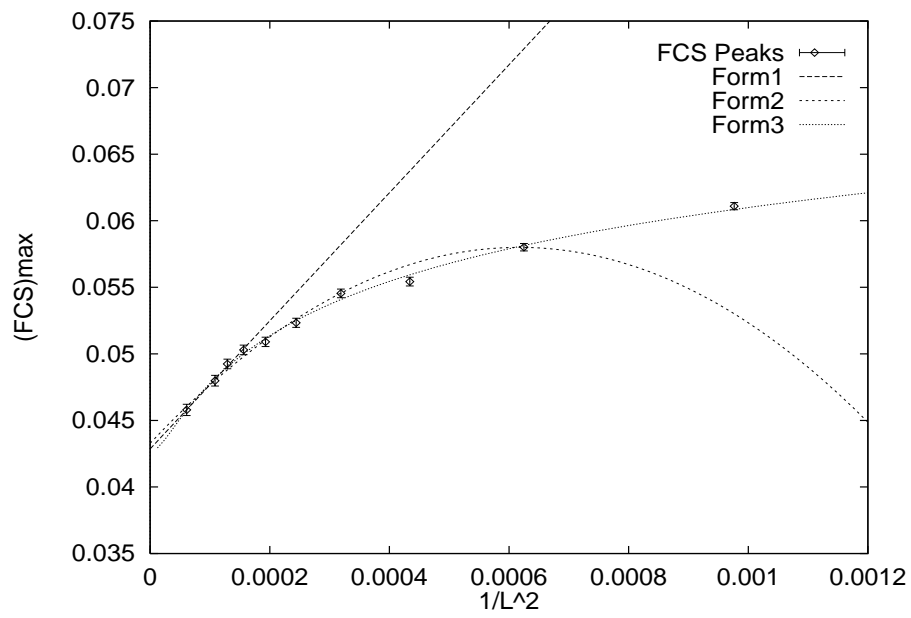


Figure 3: